

Gluconolactone
90-80-2 | DTXSID0026549

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.81 | 0.55 | 0.81 | 0.54 | 0.71 | 0.61 |

Model Results

Predicted value: 323 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.37e-01

Confidence level: 4.57e-01

Nearest Neighbors from the Training Set

| | | |
|--|---|---|
| <div>Image not found</div> <div>Glyphosate</div> <div>Measured: 2090</div> <div>Predicted: 761</div> | <div>Image not found</div> <div>Cymoxanil</div> <div>Measured: 123</div> <div>Predicted: 72.0</div> | <div>Image not found</div> <div>Glufosinate-ammonium</div> <div>Measured: 427</div> <div>Predicted: 194</div> |
| <div>Image not found</div> <div>Endothal</div> <div>Measured: 123</div> <div>Predicted: 109</div> | <div>Image not found</div> <div>Cyromazine</div> <div>Measured: 200</div> <div>Predicted: 163</div> | |